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Plasticity and Failure in Nanocrystalline BCC Metals via MD Simulation

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Abstract:
Advances in the ability to generate extremely high pressures in dynamic experiments such as at the National Ignition Facility has motivated the need for special materials optimized for those conditions as well as ways to probe the response of these materials as they are deformed. We need to develop a much deeper understanding of the behavior of materials subjected to high pressure, especially the effect of rate at the extremely high rates encountered in those experiments. Here we use large-scale molecular dynamics (MD) simulations of the high-rate deformation of nanocrystalline tantalum at pressures less than 100 GPa to investigate the processes associated with plastic deformation for strains up to 100%. We focus on 3D polycrystalline systems with typical grain sizes of 10–20 nm. We also study a rapidly quenched liquid (amorphous solid) tantalum. We apply a constant volume (isochoric), constant temperature (isothermal) shear deformation over a range of strain rates, and compute the resulting stress–strain curves to large strains for both uniaxial and biaxial compression. We study the rate dependence and identify plastic deformation mechanisms. The identification of the mechanisms is facilitated through a novel technique that computes the local grain orientation, returning it as a quaternion for each atom. This analysis technique is robust and fast, and has been used to compute the orientations on the fly during our parallel MD simulations on supercomputers. We find both dislocation and twinning processes are important, and they interact in the weak strain hardening in these extremely fine-grained microstructures. We also present some results on void growth in nanocrystalline BCC metals under tension.

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